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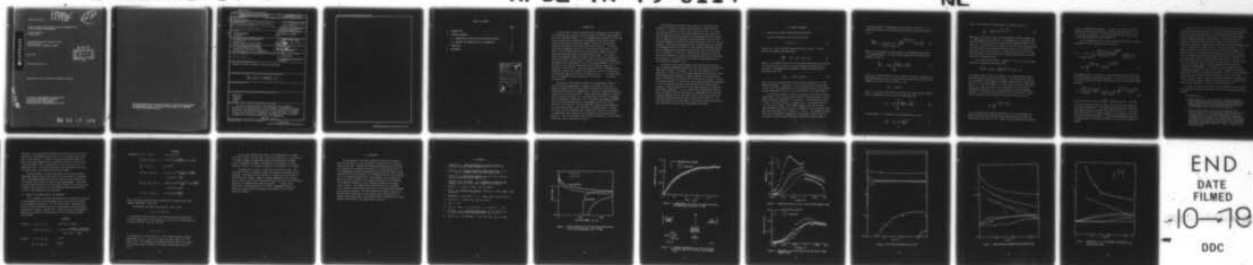
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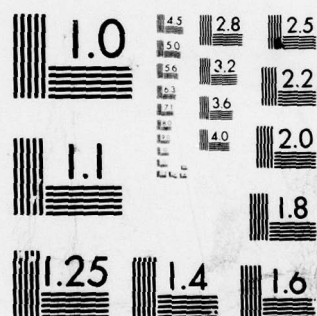
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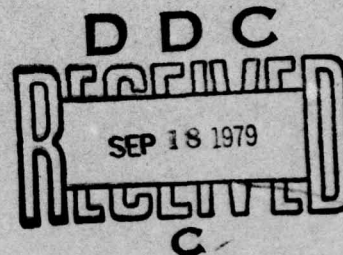
DIRECT SIMULATION MONTE CARLO DESCRIPTION
OF IONOSPHERIC CHEMISTRY

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Graham Bird

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1. INTRODUCTION

Collision theory is well established as an elementary classical theory for bimolecular gas reactions, and the concepts are readily incorporated in the direct simulation method. It is a phenomenological approach in that the binary reaction rate is obtained as the product of the kinetic theory collision rate for collisions with energy in excess of the activation energy and the probability of reaction or steric factor P_r . The steric factor may be regarded as the ratio of the reactive cross-section to the total collision cross-section and is inferred from a comparison of the theoretical prediction with the measured reaction rate. The simplest theory (for example¹) employs a constant steric factor and considers only the translational collision energy in relation to the activation energy. Refinements of the method employ a collision energy dependent steric factor and allow for the possible contribution of the internal energy of the molecules in the collision. Collision theory may also be extended to termolecular reactions (for example²) by assigning a lifetime to each binary collision and regarding the triple or ternary collision as a further binary collision between the pair of molecules in the initial collision and a third molecule.

The reaction of most obvious interest in an aerodynamic context is the dissociation-recombination of oxygen and nitrogen. These are bimolecular reactions with finite activation energies for dissociation and termolecular reactions for recombination. The direct-simulation method was applied to this reaction by Bird.³ These calculations employed a constant steric factor and the results for the dissociation rate were in agreement with the theoretical prediction. Also, the density and temperature dependence of the equilibrium state was in agreement with the law of mass action for this reaction.⁴ The gas model was, however, unrepresentative of a real diatomic gas in that there was no internal energy. A further difficulty was that computing time considerations ruled out calculations at temperatures small compared with the characteristic dissociation temperature. Similar calculations which include the effects of internal energy modes have recently been made by Larsen.⁵

Bird⁶ developed a collision theory analysis of the dissociation-recombination reaction to produce an expression for the equilibrium state that is identical in form to the law of mass action. If a particular diatomic gas is to be simulated, a comparison of the theoretical and experimental dissociation rates gives the appropriate steric factor, while a comparison of the theoretical and experimental values for the equilibrium degree of dissociation provides the binary collision lifetime parameter. The model corresponding to this extended theory was combined with Borngakke and Larsen's model⁷ for the internal energy modes and was used to compute the dissociation relaxation zone behind a strong shock wave in nitrogen.⁸ The ability to calculate the equilibrium state was particularly valuable in setting up the boundary conditions for the shock wave simulation. The simulation results were in good agreement with corresponding experimental results.

A difficulty that was encountered in the nitrogen simulation was that the negative temperature exponent in the rate equation was below the lower limit allowed in the theory. This had to be allowed for by a temperature, as well as collision energy, dependence of the steric factor. The following section presents a further extension of the bimolecular theory to include the contribution of the internal energy modes. As well as being more general, it allows much larger negative temperature exponents in the rate equations and would have coped with the accepted value for nitrogen. Unlike the existing collision theory based on the "effective square term" approach^{1,3}, it is not restricted to temperatures that are small in comparison with the characteristic temperature of the reaction. A further extension is that the model now deals with inverse power law molecules rather than being restricted to hard sphere molecules. The wider applicability of the new model is particularly useful when dealing with cases which involve a very large number of reactions.

2. TECHNICAL APPROACH

2.1 DERIVATION OF STERIC FACTORS FROM REACTION RATES

A typical bimolecular reaction may be written



where A, B, C, and D represent separate molecular species. The rate equation for species A may be written

$$-\frac{dn_A}{dt} = k_f(T) n_A n_B - k_r(T) n_C n_D. \quad (2)$$

where n is the number density with the subscripts representing the species, t is the time and $k_f(T)$ and $k_r(T)$ are the forward and reverse rate coefficients. The temperature T dependence of the rate coefficient is generally of the form

$$k(T) = a T^b \exp(-E_a/kT), \quad (3)$$

where a and b are constants, E_a is the activation energy, and k is the Boltzmann constant. The problem is to find an expression for the steric factor, or collision probability, P_r as a function of the collision energy E_c that leads explicitly to Eq. (3) in the context of collision theory.

The collision energy E_c is equal to the sum of the relative translational energy in the collision and the fraction internal energy of the two molecules that may contribute to the reaction. The translational energy is equal to $1/2 m_r c_r^2$ where $m_r = m_1 m_2 / (m_1 + m_2)$ is the reduced mass and c_r is the relative speed. The internal energy is best dealt with by specifying that the number of degrees of freedom of the two molecules that may contribute energy to the reaction is ζ_1 and ζ_2 . This number may range from zero to the number of degrees of the molecule, although there are restrictions based on angular momentum considerations on the number of

rotational degrees of freedom that can be active in a reaction.⁹ It is readily shown that, for an equilibrium gas, the distribution function of E_c/kT is

$$f\left(\frac{E_c}{kT}\right) = \frac{1}{\Gamma\left(\frac{\zeta_1 + \zeta_2}{2} + \frac{n-3}{n-1} + 1\right)} \left(\frac{E_c}{kT}\right)^{\frac{\zeta_1 + \zeta_2}{2} + \frac{n-3}{n-1}} \exp\left(-\frac{E_c}{kT}\right), \quad (4)$$

where n is the exponent of inverse power law intermolecular force and Γ is the Gamma function. Collision theory assumes that the forward rate equation is given by

$$\frac{dn_A}{dt} = -n_A v_{AB} \int_{\frac{E_a}{kT}}^{\infty} f\left(\frac{E_c}{kT}\right) P_r d\left(\frac{E_c}{kT}\right), \quad (5)$$

where v_{AB} is the equilibrium collision rate for a species A molecule with species B molecules, and E_a is the activation energy such that the reaction probability is zero for E_c less than E_a . Now

$$v_{AB} = n_B \overline{\sigma_T c_r},$$

where σ_T is the total collision cross-section and the bar denotes the mean value. A comparison of Eqs. (2) and (5) then shows that

$$k(T) = \overline{\sigma_T c_r} \int_{\frac{E_a}{kT}}^{\infty} f\left(\frac{E_c}{kT}\right) P_r d\left(\frac{E_c}{kT}\right). \quad (6)$$

For hard sphere ($n = \infty$) molecules, the standard result is that

$$\overline{\sigma_T c_r} = (d_1 + d_2)^2 \left(\frac{\pi kT}{2m_r}\right)^{1/2} \quad (7)$$

where d is the molecular diameter while, for general values of η ,

$$\overline{\sigma_T c_r} = W_{Om}^2 (K/m_r)^{\frac{2}{\eta-1}} c_r^{\frac{\eta-5}{\eta-1}}, \quad (8)$$

where W_{Om} is the cut-off value of the dimensionless impact parameter and K is the constant in the force law. The parameter W_{Om} is related to the lower cut-off value that must be chosen for the deflection angle in the collision. The value of P_r will depend on this choice and the generalized collision theory is unsatisfactory when the overall aim is merely the calculation of the steric factor P_r . However, this is not a difficulty when this factor is used in the direct simulation method since a cut-off value must be specified anyway.

If a constant steric factor is employed in Eq. (6), it may be taken outside the integration which then yields

$$\Gamma\left(\frac{\zeta_1 + \zeta_2}{2} + \frac{\eta-3}{\eta-1} + 1, \frac{E_a}{kT}\right) / \Gamma\left(\frac{\zeta_1 + \zeta_2}{2} + \frac{\eta-3}{\eta-1} + 1\right).$$

For integer values of the first argument, the incomplete Gamma function may be written as a power series in E_a/kT . This is effectively done in the "activation in many degrees of freedom" theory¹ and the "square term" theory.⁴ All but the leading term of the power series may be discarded when $kT \ll E_a$ but, while this is satisfactory for the dissociation-recombination reaction, it is out of the question for fast exothermic reactions. This problem may be avoided by the introduction of a steric factor proportional to some power of $E_c - E_a$ multiplied by the term

$$\left(1 - \frac{E_a}{E_c}\right)^{\frac{\zeta_1 + \zeta_2}{2} + \frac{\eta-3}{\eta-1}}.$$

This term enables the incomplete Gamma function to be transformed to a Gamma function that does not involve the temperature, and leads to the desired form of Eq. (3) for $k(T)$. Moreover, this modification has physical

as well as mathematical advantages. It means that P_r need no longer be constant for very large values of E_c and the rise from zero at $E_c = E_a$ is no longer discontinuous. Similar forms for the steric factor have, in fact, been proposed for these reasons.^{1,10}

The full expression for the steric factor that yields Eq. (3) when substituted into Eq. (6) with Eqs. (4) and (8) is

$$P_r = \frac{\epsilon}{2\pi^{1/2} W_{0m}^2 (k/m_e)^{1/2}} \frac{\Gamma\left(\frac{\zeta_1 + \zeta_2}{2} + \frac{\eta-3}{\eta-1} + 1\right)}{\Gamma[2(\eta-2)/(\eta-1)]} \left(\frac{m_r}{2K}\right)^{\frac{\eta-5}{2(\eta-1)}} \frac{a}{\Gamma\left(\frac{\zeta_1 + \zeta_2}{2} + \frac{3}{2} + b\right)} \cdot \left(1 - \frac{E_a}{E_c}\right)^{\frac{\zeta_1 + \zeta_2}{2} + \frac{\eta-3}{\eta-1}} \left(\frac{E_c - E_a}{k}\right)^{b - \frac{\eta-5}{2(\eta-1)}} \quad (9)$$

The symmetry factor ϵ is equal to 1 for unlike molecules and 2 when both collision partners are of the same species. The use of Eq. (7) in place of Eq. (8) gives the following simplified form of Eq. (9) for hard sphere molecules:

$$P_r = \frac{\Gamma\left(\frac{\zeta_1 + \zeta_2}{2} + 2\right)}{(d_1 + d_2)^2} \left(\frac{2m_r}{\pi k}\right)^{1/2} \frac{a}{\Gamma\left(\frac{\zeta_1 + \zeta_2}{2} + \frac{3}{2} + b\right)} \left(1 - \frac{E_a}{E_c}\right)^{\frac{\zeta_1 + \zeta_2}{2} + 1} \left(\frac{E_c - E_a}{k}\right)^{b-1/2} \quad (10)$$

The minimum value of b is now $-\left(\frac{\zeta_1 + \zeta_2}{2} + \frac{3}{2}\right)$ rather than the $-\frac{3}{2}$ allowed by earlier theory which does not take into account the contribution of the internal energy modes. The extended theory would have covered the experimental values for nitrogen that caused difficulties in the shock wave calculations.⁸ This general behavior is consistent with the more restricted "square term" theory, in that increasing negative value of b are associated with a greater contribution from the internal degrees of freedom.

The use of Eqs. (9) or (10) to obtain the steric factor for use in a simulation program ensures that the reaction rates will agree with those from the continuum rate equation in flow situations where near translational and rotational equilibrium prevail and both the discrete particle and the continuum approaches are applicable. The discrete particle approach, through the direct-simulation method, permits results to be obtained for chemically reacting flow situations with marked non-equilibrium in the translational and internal modes. The critical question is the degree of realism in the modeling of the real flow in this regime. It should be kept in mind that the above equations for the collision probability constitute phenomenological models which are not unique and which have been based largely on considerations of mathematical tractability. The ideal would be to have tabulations of reaction cross-sections as functions of the energy states and impact parameters based on quantum calculations and experiment. The progress in this direction has been reviewed by Toennies,¹¹ and very little of this information is currently available for reactions of engineering interest. When a classical approach based primarily on continuum rate data must be used, the above model appears to offer the most practical approach for chemically reacting flows in the transition regime. Hopefully, the physical basis is sufficiently sound for the predictions to be at least qualitatively valid.

In order to consider the direct simulation method as an alternative to conventional continuum calculations, the following conditions should be assessed.

The advantages are:

- The gas need not be in an equilibrium or quasi-equilibrium state. Not only may each species have a separate temperature, but the velocity distributions functions may vary drastically from the Maxwellian distribution and the internal modes may be out of equilibrium with the translational mode.
- The calculations make direct use of the reactive cross-sections as functions of the molecular properties and collision impact parameters. The fact that these do not have to be averaged to give rate constants as a function of temperature is particularly advantageous for electron-neutral and electron-ion reactions for which the cross-section versus energy curves often have closely spaced peaks and valleys. The vibrational states may be regarded as reactions. Radiative reactions may also be included.

The disadvantages are:

- The number of representative simulated modules is generally restricted to some thousands and the total number of simulated collisions to some millions. This means that it is impractical to simulate reactions which occur less frequently than once every thousand elastic collisions (i.e., steric factors less than about 10^{-3}). This rules out some very slow bimolecular reactions and generally rules out termolecular reactions.
- There are sampling difficulties associated with trace species, although these may be alleviated, to some extent, through the use of weighting factors such that the number of real molecules represented by each simulated molecule varies from species to species.
- Most of the currently available data is presented as rate coefficients as a function of temperature, rather than as reactive cross-sections as a function of the collision energy. This data must be analytically converted to give the same answer in the quasi-equilibrium situations for which the continuum approach is valid. (The magnitude of the steric factors given by this conversion process provides a useful check on the physical validity of the rate data.)

The above considerations lead to the conclusion that direct molecular simulation is most suitable for rapidly varying transient phenomena in the upper regions of the atmosphere. It can be used in situations where the conventional continuum approach would be invalid.

Illustrative Example

The direct simulation method has been applied to the vibrational excitation of steam. The reason for choosing steam is that it has¹² an anomalously rapid vibrational relaxation rate for V-T collisions. The scatter in the data is such that the temperature exponent is uncertain and a constant value of $3.5 \times 10^{-17} \text{ m}^3 \text{ s}^{-1}$ per molecule has been used for the deactivation rate. The characteristic temperature of the reaction is 2293K so that the activation rate coefficient given by the product of the deactivation coefficient and $\exp(-2295/T)$. The resulting steric factors from Eq. (10) are shown in Figure 1.

A homogeneous relaxation case was computed for initial conditions of $T = 650\text{K}$, $n = 10^{23} \text{ m}^{-3}$ and $n^* = 0$. Here, n and n^* are the number densities of the ground state and first vibrational level, respectively. Eq. (2) becomes

$$\frac{d}{dt} \left(\frac{n^*}{n} \right) = 3.5 \times 10^6 \left[\exp - \left(\frac{2295}{T} \right) - \frac{n^*}{n} \right] \quad (11)$$

and energy conservation requires,

$$T = 650 - 918 (n^*/n) . \quad (12)$$

Figure 2 compares the simulation results with a numerical solution of eqs. (11) and (12). The two are in good agreement even though this is a sufficiently fast reaction for a substantial departure from local translational and rotational equilibrium to be expected. The equilibrium concentration ratio is also in good agreement with the equilibrium value even though the simulation procedures based on collision theory cannot be expected to satisfy detailed balancing.

In order to illustrate the effects of translational equilibrium in a transition regime flow, the steam model was then applied to the steady flow through a screen or grid. This flow is schematically represented in Figure 3 which also defines the flowfield dimensions and the initial and boundary conditions. This is a one-dimensional flow in which the grid is a hypothetical device which reflects a specified percentage of the molecules passing through it. The initial temperature was chosen such that the initial equilibrium excitation is negligible and the grid solidity is sufficiently large to produce a temperature with a significant degree of equilibrium excitation. The temperature profiles along this flow ahead of the grid shown in Figure 4 are very similar to those for a normal shock wave. There is a temperature jump at the grid location and, since the downstream Mach number in this flow is barely supersonic, there is some upstream influence from the open end. The parallel temperature T_x based on the velocity components in the flow direction overshoots the overall temperature T by a significant margin. The normal temperature T_n based on the other components overshoots T by a small margin, while the rotational temperature T_r lags behind T .

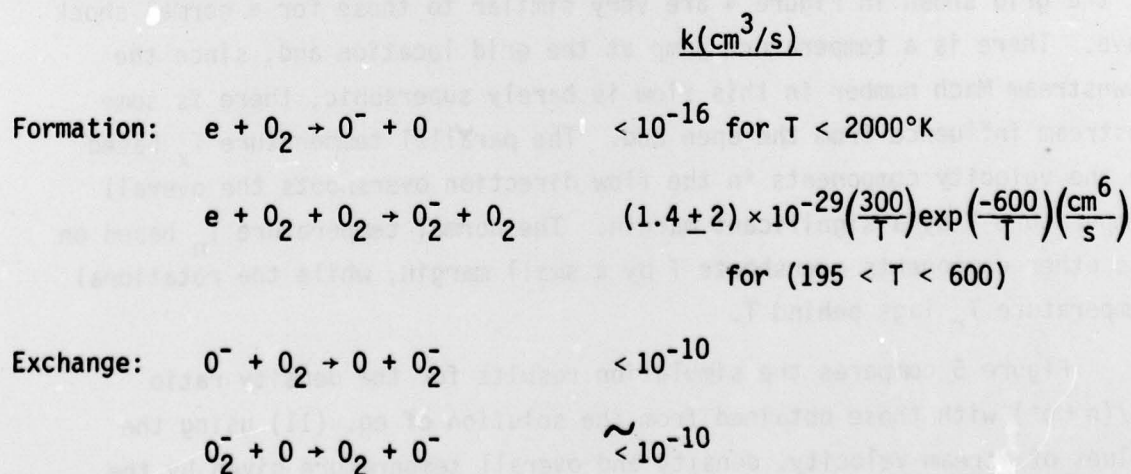
Figure 5 compares the simulation results for the density ratio $n^*/(n+n^*)$ with those obtained from the solution of eq. (11) using the values of stream velocity, density and overall temperature given by the

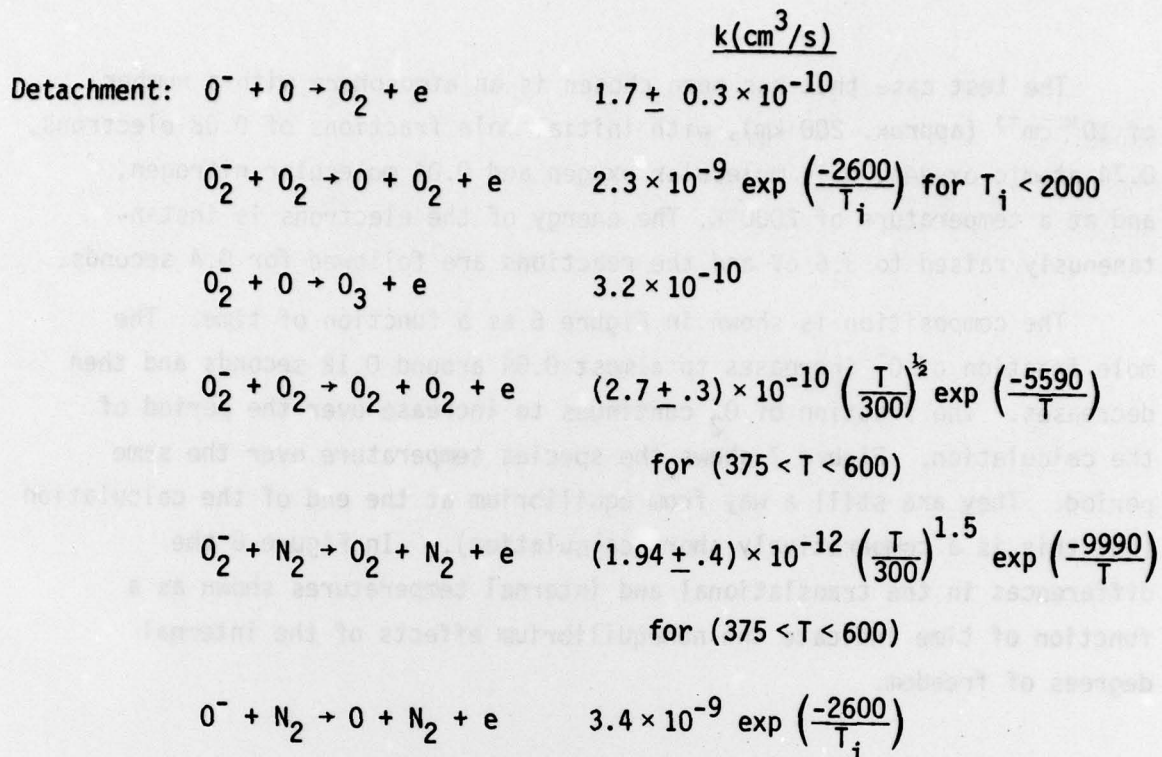
simulation. The non-equilibrium effects are significant and, as would be expected from the temperature profiles in Fig. 4, they are greater when the collision energy E_c is obtained from the translational modes only. Other calculations showed that the vibrational overshoot is much larger if the rate coefficient is proportional to a finite positive power of temperature, but is not greatly affected by the replacement of the basic hard sphere model by an inverse ninth power law model.

The above example illustrates the scope of the direct-simulation method when chemical data is available only in the form of bulk reaction rates. Approximate quantum cross-section predictions are available for T-V reactions such as that for steam in the second example. The direct-simulation approach would also be particularly useful for the reverse task of deducing rate coefficients or even flowfields from these predictions in order to make comparisons with experiment.

2.2 NEGATIVE ION COMPOSITION IN THE IONOSPHERE

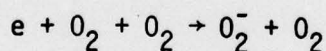
A set of chemical reactions representative of the important processes in the ionosphere has been investigated by the direct simulation Monte Carlo method described earlier. In this calculation, a homogeneous gas mixture initially containing electrons, atomic oxygen, molecular oxygen, and molecular nitrogen. Equation (10) is used to convert the temperature dependent rate coefficients given below to collision energy dependent steric factors.



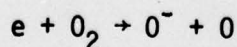


Most of the rate coefficients were obtained from the DNA Reaction Rate Handbook (DNA.19484), March 1972.

Two formation reactions are considered. One of these



is a termolecular reaction with a rate coefficient that indicates that it occurs only once every 10^7 binary O_2 , O_2 collisions at a number density of 10^9 to 10^{10} cm^{-3} . The other reaction



is bimolecular but, being dissociative, has a high activation energy of approximately 3.6 eV. Above this energy, the steric factor is of the order of 0.2. The exchange and detachment reactions have steric factors, in the energy range of interest, that range from the order of 10^{-3} to unity.

The test case that has been chosen is an atmosphere with a number of 10^{10} cm^{-3} (approx. 200 km), with initial mole fractions of 0.08 electrons, 0.74 atomic oxygen, 0.14 molecular oxygen and 0.04 molecular nitrogen, and at a temperature of 2000°K. The energy of the electrons is instantaneously raised to 3.6 eV and the reactions are followed for 0.4 seconds.

The composition is shown in Figure 6 as a function of time. The mole fraction of O^- increases to almost 0.04 around 0.12 seconds and then decreases. The fraction of O_2^- continues to increase over the period of the calculation. Figure 7 shows the species temperature over the same period. They are still a way from equilibrium at the end of the calculation (but this is a comparatively short calculation). In Figure 8 the differences in the translational and internal temperatures shown as a function of time indicate the nonequilibrium effects of the internal degrees of freedom.

3. CONCLUSION

The application of the direct simulation Monte Carlo method to describe the chemistry in the ionosphere is potentially a very useful computational tool. Although the calculations presented are restricted to a reaction cell simulation where there are no spatial gradients in the thermodynamic variables the method does describe the effects of the electrons and ions and nonequilibrium influences which are not accounted for in the continuum descriptions. The procedure can be used to parametrically study the effect of high energy electrons on the chemistry of the ambient ionosphere or as a screening procedure for possible reaction chains. This computational procedure will be incorporated in the future into the general Monte Carlo ion collection code developed under previous contracts. The resulting code will then be capable of describing the disturbance of the ionosphere due to the passage of a charged rocket borne probe, including the effects of molecular collisions, electric field effects, and nonequilibrium chemistry.

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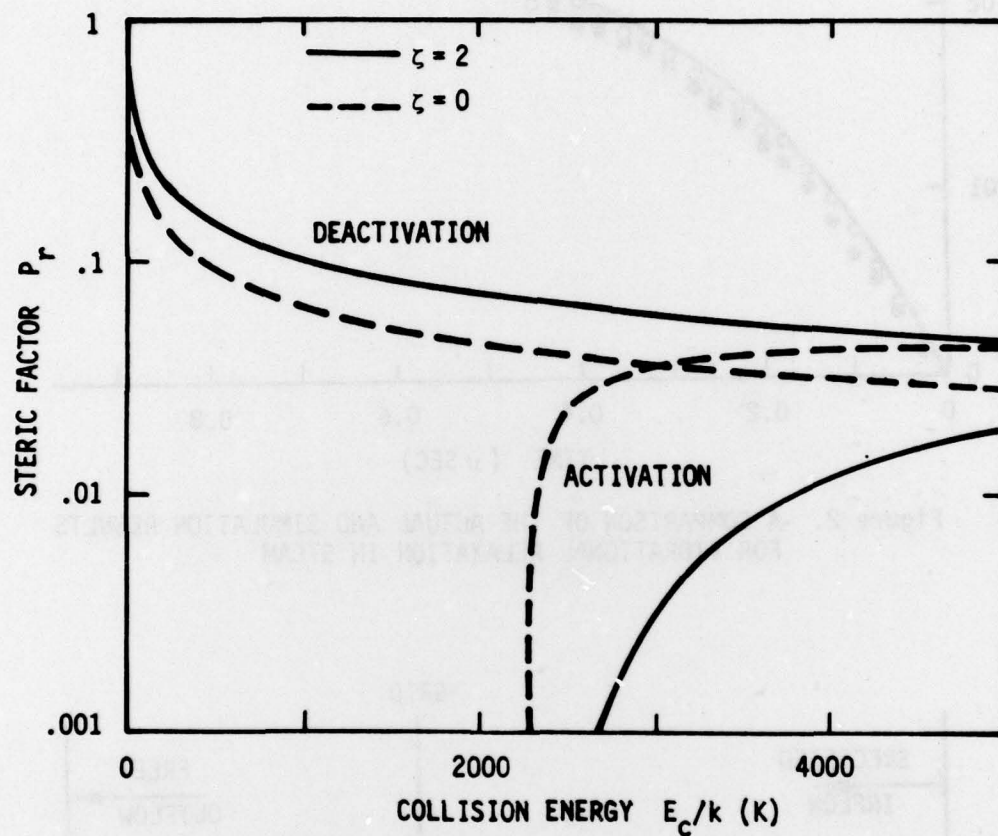


Figure 1. STERIC FACTORS FOR THE ACTIVATION AND DEACTIVATION OF THE FIRST VIBRATIONAL LEVEL IN STEAM

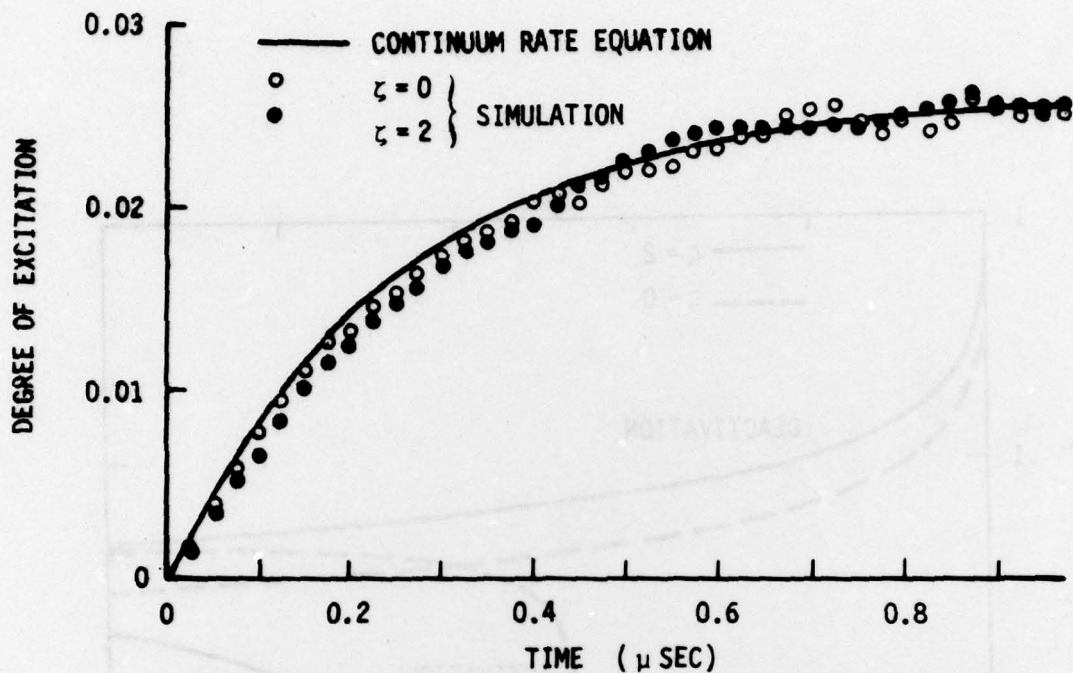


Figure 2. A COMPARISON OF THE ACTUAL AND SIMULATION RESULTS FOR VIBRATIONAL RELAXATION IN STEAM

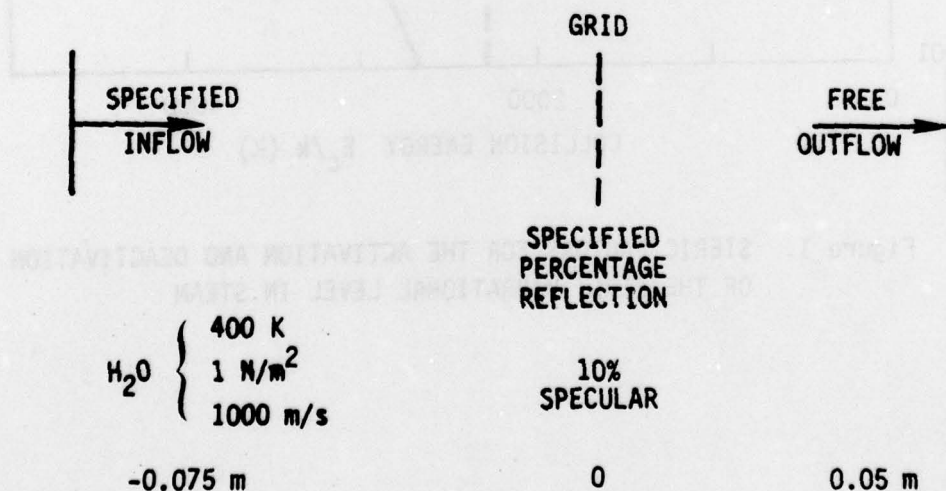


Figure 3. A SCHEMATIC REPRESENTATION AND DATA DEFINITION OF THE TEST CASE FOR THE FLOW OF STEAM THROUGH A GRID

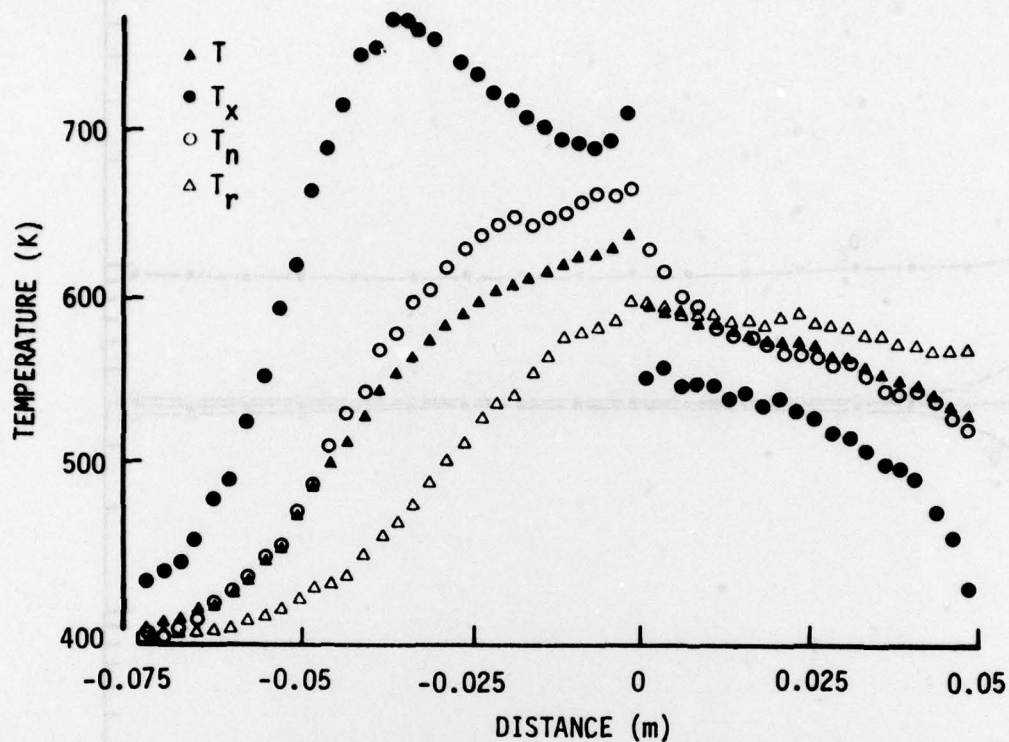


Figure 4. TEMPERATURE PROFILES FOR THE FLOW OF STEAM THROUGH A GRID

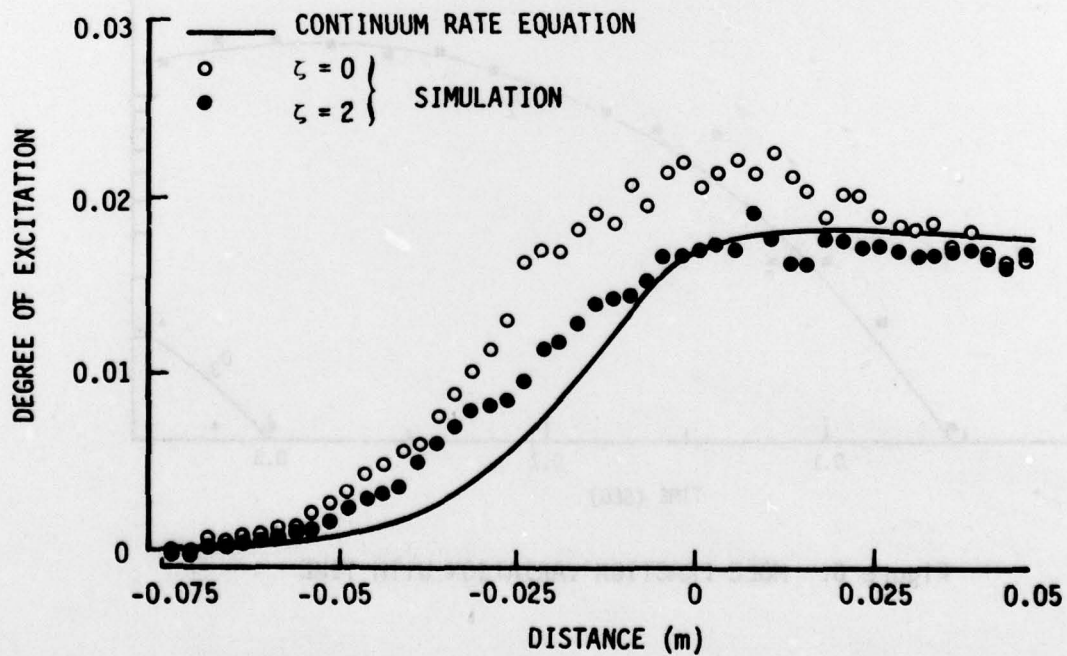


Figure 5. VIBRATIONAL EXCITATION PROFILES FOR THE FLOW OF STEAM THROUGH A GRID

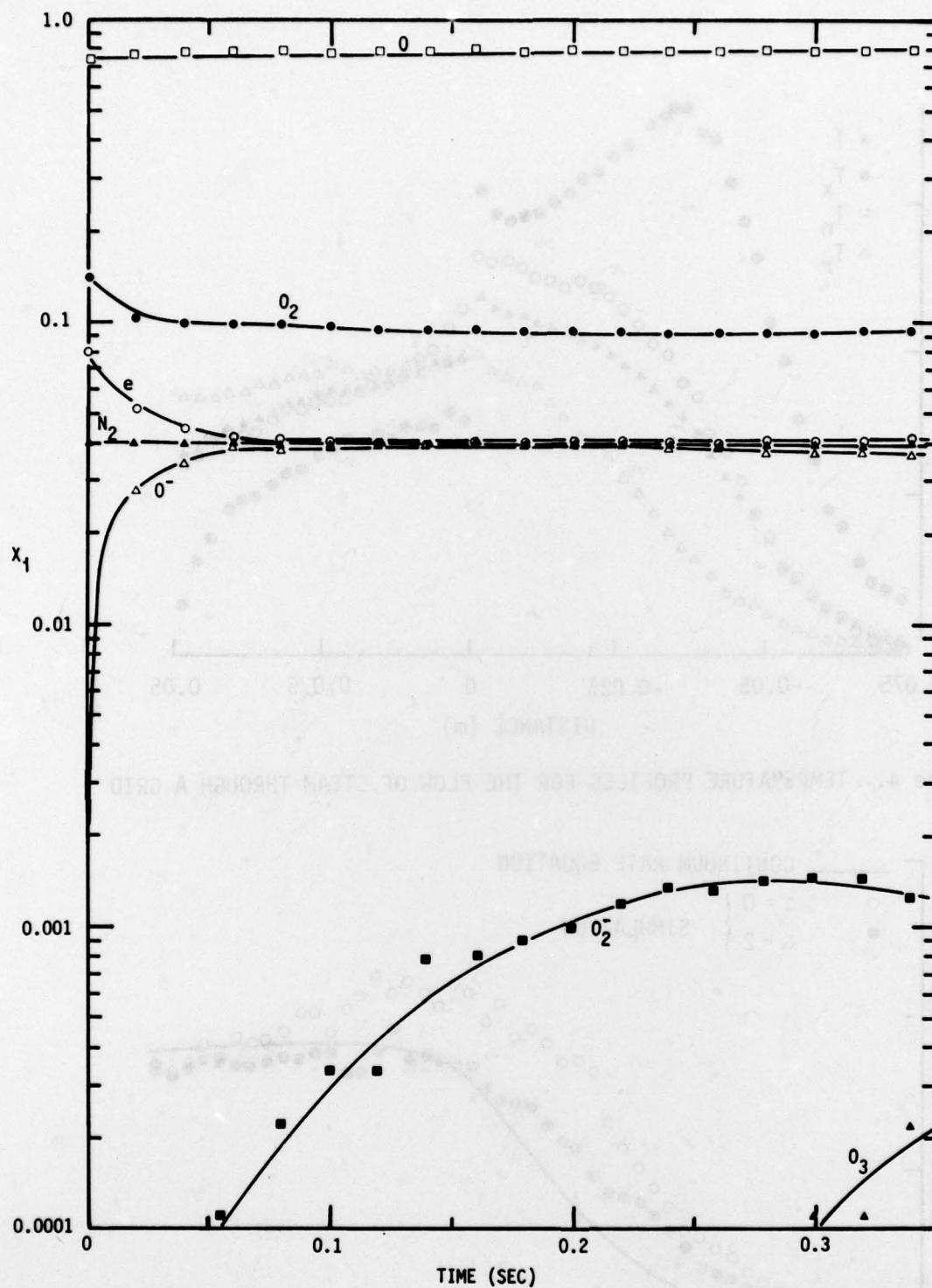


Figure 6. MOLE FRACTION VARIATION WITH TIME

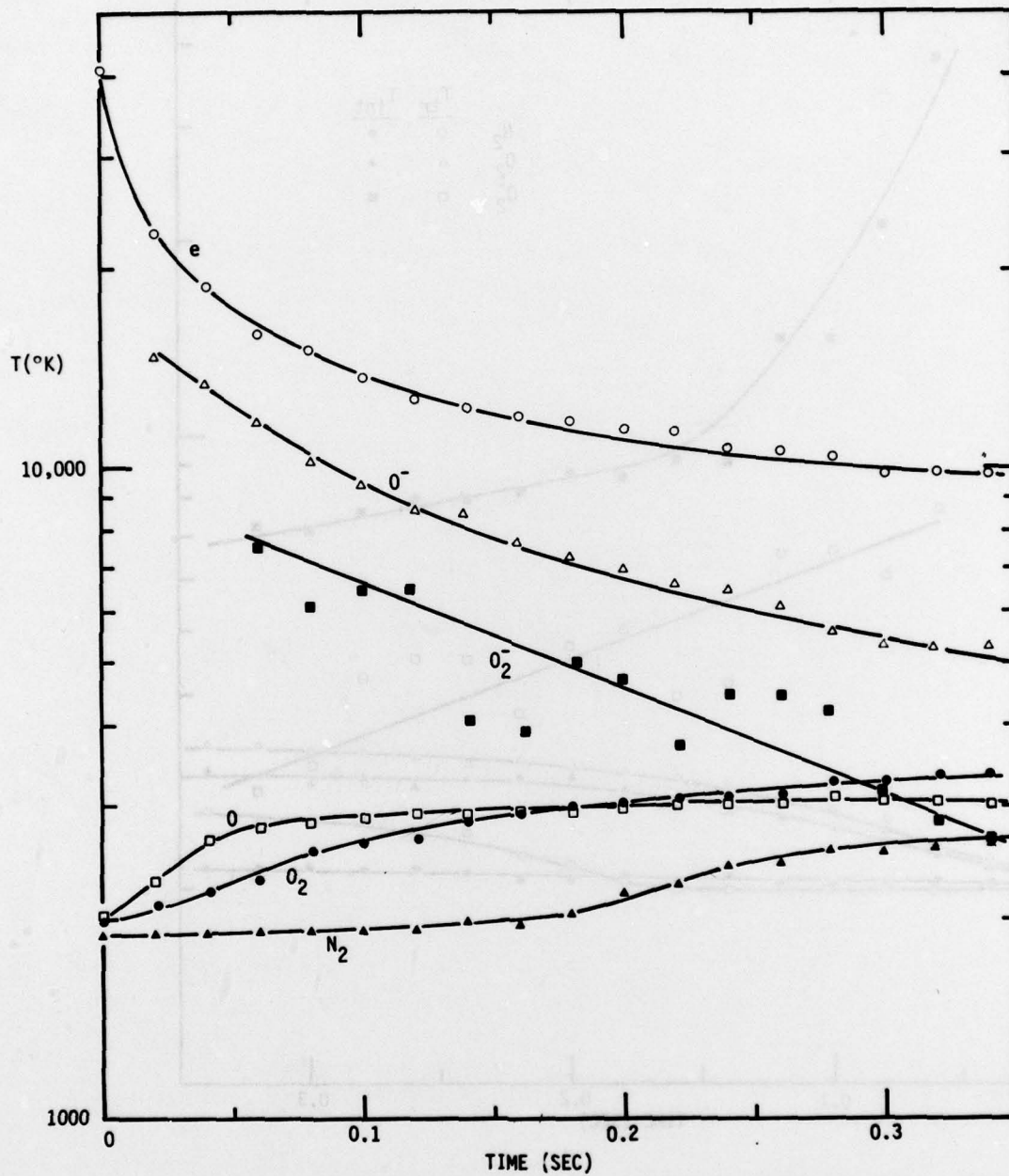


Figure 7. TRANSLATIONAL TEMPERATURE VARIATION WITH TIME

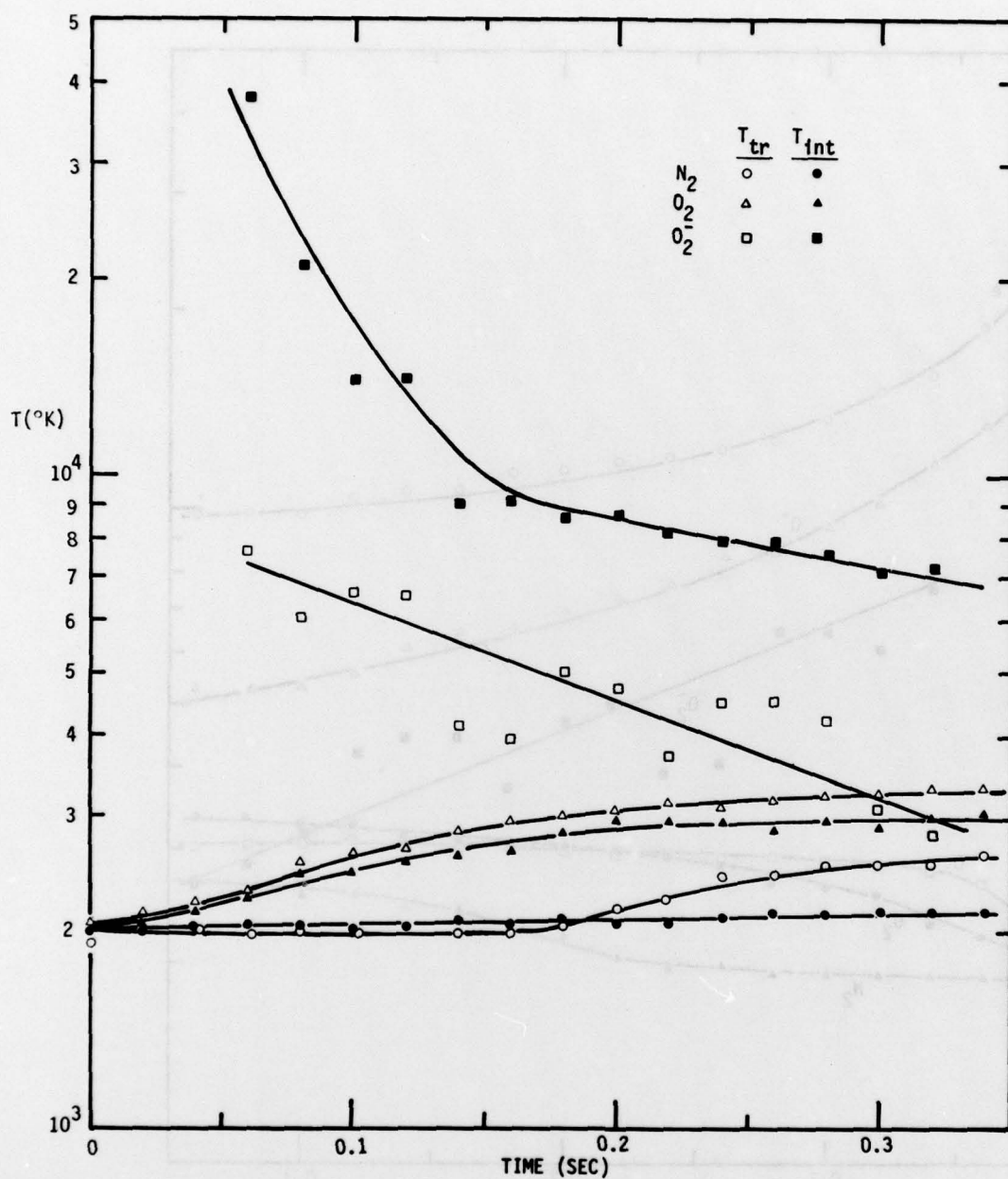


Figure 8. TRANSLATIONAL (T_{tr}) AND INTERNAL TEMPERATURE (T_{int}) VARIATION WITH TIME